

74
180/p6

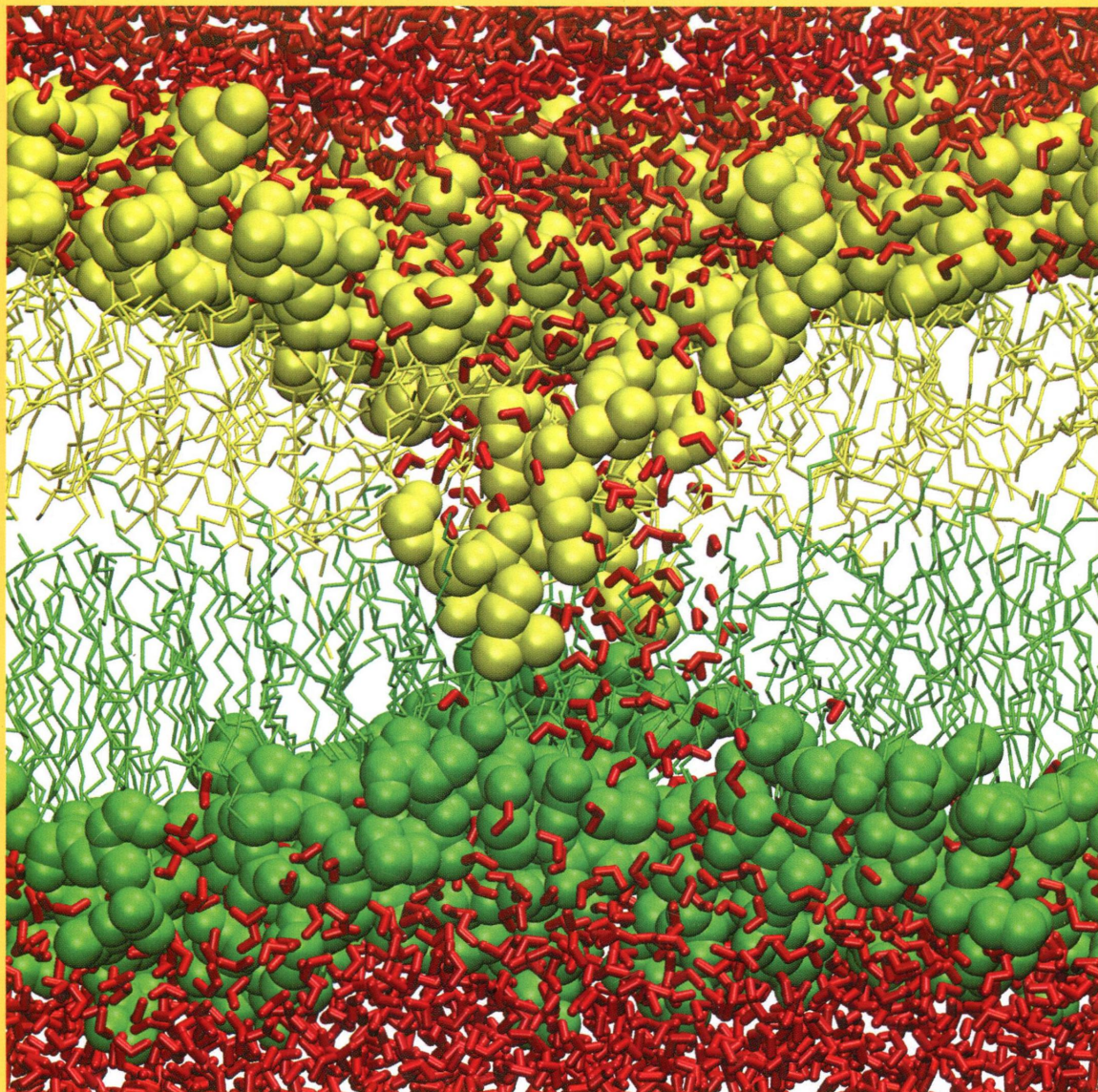
AUGUST 21, 2014

VOLUME 118

NUMBER 33

pubs.acs.org/JPCB

THE JOURNAL OF PHYSICAL CHEMISTRY

B

**Electric Field-Induced
Pore Formation
in an Asymmetric
Model Membrane
Comprised of
Phosphatidylcholine
(Yellow) and
Phosphatidyl-
ethanolamine (Green)
Lipid Monolayers
(see page 9909)**

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

ON THE COVER: Electric field-induced pore formation in an asymmetric model membrane comprised of phosphatidylcholine (yellow) and phosphatidylethanolamine (green) lipid monolayers. Electroporation phenomena in asymmetric phospholipid membranes. Atomic-scale molecular dynamics simulations reveal the molecular mechanism of electric field-induced pore formation in asymmetric membranes comprised of phosphatidylcholine (PC) and phosphatidylethanolamine (PE) lipid monolayers. Such model membranes account for the transmembrane lipid asymmetry that is an inherent feature of plasma membranes of animal cells: PC and PE lipid monolayers mimic the outer and inner leaflets of plasma membranes, respectively. The cover displays an early stage of pore formation in an asymmetric PC/PE membrane as induced by an external electric field. In contrast to single-component phospholipid membranes, the formation of a pore turns out to be asymmetric and occurs mainly on the PC side. In particular, water molecules penetrate in the membrane interior mostly from the PC side and the reorientation of lipid head groups also takes place in the PC leaflet. In turn, the PE leaflet is considerably more robust against an electric field due to inter-lipid hydrogen bonding, so that the PE lipid head groups do not enter the central region of the membrane till the water pore becomes rather large and is partly stabilized by PC head groups. Overall, the findings provide compelling evidence that the transmembrane lipid asymmetry can be essential for understanding electroporation phenomena in living cells. PC and PE lipids are shown in yellow and green, respectively; water molecules are shown in red. See page 9909.

Articles

Biophysical Chemistry and Biomolecules

9819

[dx.doi.org/10.1021/jp503227j](https://doi.org/10.1021/jp503227j)

Free Radical Scavenging Properties of Phytofluene and Phytoene Isomers as Compared to Lycopene: A Combined Experimental and Theoretical Study

Ana Martínez,* Carla M. Stinco, and Antonio J. Meléndez-Martínez

9826

[dx.doi.org/10.1021/jp5034245](https://doi.org/10.1021/jp5034245)

Hot Spot of Structural Ambivalence in Prion Protein Revealed by Secondary Structure Principal Component Analysis

Norifumi Yamamoto*

9834



[dx.doi.org/10.1021/jp504201k](https://doi.org/10.1021/jp504201k)

New Insight into Amyloid Fibril Formation of Hen Egg White Lysozyme Using a Two-Step Temperature-Dependent FTIR Approach


Ye Zou, Wenying Hao, Haoyi Li, Yachao Gao, Ying Sun, and Gang Ma*

9844

[dx.doi.org/10.1021/jp504243e](https://doi.org/10.1021/jp504243e)

Effects of Galactosylation in Immunoglobulin G from All-Atom Molecular Dynamics Simulations

Michael E. Fortunato and Coray M. Colina*

9852  [dx.doi.org/10.1021/jp504516a](https://doi.org/10.1021/jp504516a)

Computational Investigation of Cholesterol Binding Sites on Mitochondrial VDAC

Brian P. Weiser, Reza Salari, Roderic G. Eckenhoff, and Grace Brannigan*

9861  [dx.doi.org/10.1021/jp505400q](https://doi.org/10.1021/jp505400q)

Conformational and Thermodynamic Properties of Non-Canonical α,α -Dialkyl Glycines in the Peptaibol Alamethicin: Molecular Dynamics Studies

Tarsila G. Castro and Nuno M. Micaêlo*

9871  [dx.doi.org/10.1021/jp505638w](https://doi.org/10.1021/jp505638w)

The Influence of Ser-154, Cys-113, and the Phosphorylated Threonine Residue on the Catalytic Reaction Mechanism of Pin1

Esteban Vöhringer-Martinez,* Toon Verstraelen, and Paul W. Ayers

9881  [dx.doi.org/10.1021/jp505643w](https://doi.org/10.1021/jp505643w)

Origins of Structural Flexibility in Protein-Based Supramolecular Polymers Revealed by DEER Spectroscopy

Nathan A. Tavenor, K. Ishara Silva, Sunil Saxena,* and W. Seth Horne*

9890  [dx.doi.org/10.1021/jp506211b](https://doi.org/10.1021/jp506211b)

Structural and Functional Stability of Cellulase in Aqueous-Biomphiphilic Ionic Liquid Surfactant Solution

Pankaj Bharmoria, Mohit J. Mehta, Imran Pancha, and Arvind Kumar*

Biomaterials, Surfactants, and Membranes

9900  [dx.doi.org/10.1021/jp5020077](https://doi.org/10.1021/jp5020077)

Fibronectin Module FN^{III}9 Adsorption at Contrasting Solid Model Surfaces Studied by Atomistic Molecular Dynamics

Karina Kubiak-Ossowska, Paul A. Mulheran,* and Wieslaw Nowak

9909 [dx.doi.org/10.1021/jp5028355](https://doi.org/10.1021/jp5028355)

Electroporation of Asymmetric Phospholipid Membranes

Andrey A. Gurtovenko* and Anastasia S. Lyulina

Liquids; Chemical and Dynamical Processes in Solution

9919 [dx.doi.org/10.1021/jp5043975](https://doi.org/10.1021/jp5043975)


Local Hydration Pressures in Methanol Aqueous Solution: A Raman Spectroscopy Analysis


Nubia Judith Mendoza, Laura Jiménez Bonales, Valentin Garcia Baonza, and Mercedes Cáceres*

9926  [dx.doi.org/10.1021/jp504631n](https://doi.org/10.1021/jp504631n)

Analyte Interactions with a New Ditopic Dansylamide–Nitrobenzoxadiazole Dyad: A Combined Photophysical, NMR, and Theoretical (DFT) Study

Abhas Kumar Bhoi, Sudhir Kumar Das, Debashis Majhi, Prabhat Kumar Sahu, A. Nijamudheen, Anoop N., Abdur Rahaman, and Moly Sarkar*

9938  [dx.doi.org/10.1021/jp505129m](https://doi.org/10.1021/jp505129m)
Electronic Structure of Hemin in Solution Studied by Resonant X-ray Emission Spectroscopy and Electronic Structure Calculations
Kaan Atak, Ronny Golnak, Jie Xiao, Edlira Suljoti, Mika Pflüger, Tim Brandenburg, Bernd Winter, and Emad F. Aziz*

9944  [dx.doi.org/10.1021/jp505592t](https://doi.org/10.1021/jp505592t)
Physicochemical and Thermal Properties for a Series of 1-Alkyl-4-methyl-1,2,4-triazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquids
Andrea T. De La Hoz, Ulises G. Brauer, and Kevin M. Miller*

9952  [dx.doi.org/10.1021/jp506062j](https://doi.org/10.1021/jp506062j)
Excited-State Dynamics of an Environment-Sensitive Push–Pull Diketopyrrolopyrrole: Major Differences between the Bulk Solution Phase and the Dodecane/Water Interface
Sabine Richert, Sandra Mosquera Vazquez, Marek Grzybowski, Daniel T. Gryko, Alexander Kyrychenko, and Eric Vauthey*

9964  [dx.doi.org/10.1021/jp506572p](https://doi.org/10.1021/jp506572p)
Dynamic Solvation Shell and Solubility of C₆₀ in Organic Solvents
Chun I Wang, Chi C. Hua,* and Show A. Chen


Glasses, Colloids, Polymers, and Soft Matter

9974 [dx.doi.org/10.1021/jp504450h](https://doi.org/10.1021/jp504450h)
Factors Influencing Crystal Growth Rates from Undercooled Liquids of Pharmaceutical Compounds
Niraj S. Trasi, Jared A. Baird, Umesh S. Kestur, and Lynne S. Taylor*

9983 [dx.doi.org/10.1021/jp504998t](https://doi.org/10.1021/jp504998t)
Amphiphilic Self-Assembly of Alkanols in Protic Ionic Liquids
Haihui Joy Jiang, Paul A. FitzGerald, Andrew Dolan, Rob Atkin, and Gregory G. Warr*

9991  [dx.doi.org/10.1021/jp505133q](https://doi.org/10.1021/jp505133q)
Structure of Intermediate Phase II of LiNH₂ under High Pressure
Hiroshi Yamawaki,* Hiroshi Fujihisa, Yoshito Gotoh, and Satoshi Nakano

9997 [dx.doi.org/10.1021/jp5067956](https://doi.org/10.1021/jp5067956)
Radical–Triplet Pair Interactions as Probes of Long-Range Polymer Motion in Solution
Sooyeon Sim and Malcolm D. E. Forbes*

 Supporting Information available via online article